Scalable Linear Solvers (Rob Falgout, PI)

At the core of many DOE simulation codes is the need to solve huge linear systems on thousands of processors. Multigrid methods are so-called scalable or optimal methods because they can solve a linear system with N unknowns with only O(N) work. This property makes it possible to solve ever larger problems on proportionally larger parallel machines in constant time. LLNL researchers are working on algebraic multigrid/(AMG) approaches that are well suited for addressing a variety of problems that are challenging or impossible to solve using the classical multigrid approach. Our main accomplishment this past year concerns the scalable solution of the definite Maxwell's equations. The major difficulty with developing scalable solvers for these equations is the oscillatory, huge near null space and the fact that such problems are often solved on unstructured grids. Previous attempts to construct AMG methods have had only partial success. Our new auxiliary-space Maxwell solver (AMS) is based on our previous work on auxiliary mesh preconditioners and the Hiptmair/Xu solver which does not require an explicit remeshing of the problem on a uniform mesh. Our new AMS solver is an improved version of the Hiptmair/Xu solver and is the first provably scalable solver for the definite Maxwell's equations on quasi-uniform unstructured meshes that requires minimal additional information from the user.

Parallel Electromagnetics Solvers (Bill Henshaw, PI)

LLNL researchers have developed a new approach for the fast and efficient simulation of electromagnetic phenomena on parallel computers.
The new technique enables the accurate solution of Maxwell's equations for complex geometry, with potential to impact a wide range of applications such as high-energy particle accelerators, digital circuits and optical telecommunications. The new scheme for solving Maxwell's equations uses overlapping grids, with narrow curvilinear grids fitted to boundaries and interfaces, coupled to Cartesian grids that occupy most of the domain. This approach combines the efficiency of methods for Cartesian grids with the flexibility and accuracy for complex geometry of methods based on unstructured grids. Our scheme uses new high-order accurate symmetric approximations for general curvilinear grids that exactly preserve the electromagnetic energy. Unlike many finite element approximations that require the inversion of an implicit mass matrix, these symmetric schemes are fully explicit and efficient to evaluate. A key component of the new scheme is the construction of centered, high-order accurate approximations at material interfaces and the development of the mathematical theory to support the properties of these discrete approximations that allow the interface to be treated to high-order accuracy even though the solution and its derivatives can be discontinuous at the interface. This work has been used in collaboration with Dr. Kwok Ko at SLAC to compute an electromagnetic pulse in a key component of the proposed International Linear collider.

Serpentine (Anders Petersson, PI)

Simulation of wave propagation phenomena is essential for the success of many DOE programs such as strong ground motion prediction for the Enhanced Test Site Readiness Program, the Yucca Mountain Program, underground explosion monitoring and underground facilities characterization. During the past year, LLNL researchers developed new numerical simulation capabilities for seismic wave propagation modeled by the three-dimensional elastic wave equation in domains with complex material properties and subject to stress-free boundary conditions. The second order formulation of the elastic wave equation was discretized using a summation-by-parts technique which guarantees a robust numerical scheme that is stable even when the material properties vary arbitrarily from point to point in the computational mesh. The new technique improves on previous numerical schemes by being second order accurate, energy conserving, and stable for all ratios between the longitudinal and transverse wave speeds. This method was used to simulate an extended earthquake rupture on the San Andreas fault modeling the great San Francisco earthquake in 1906. The calculations, which were run on up to
1024 processors on a LLNL linux cluster, produced state-of-the-art predictions of the ground motion using up to 4 billion grid points covering all of northern California.

Deformable Boundaries (Petri Fast, PI)

Advanced algorithms development at LLNL enabled new reference simulations of unprecedented scale for the Saffman-Taylor (ST) "viscous fingering" instability. Viscous fingering is a prototypical free-boundary problem that shares many of the difficulties often encountered in simulations of dynamic boundaries in fluids. These simulations illustrate the effect Moore's law has on simulations of fluid dynamic interfacial instabilities: While computing power has increased 100 times in the past ten years, far more important has been the discovery of algorithms with optimal runtime complexity under Office of Science funding. Improvements in algorithms for studying fluid dynamic instabilities are of central importance to the DOE mission.
Simulations using the new algorithms reached a new asymptotic scaling regime that can be matched to an experimentally measured power-law characterization of the evolving interfacial shape. Such simulations would have been impossible using previously developed algorithms, even on today's supercomputers.

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